

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
 Data File : BG055271.D
 Acq On : 25 Oct 2022 11:12
 Operator : CG/JU
 Sample : N5253-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 124055

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.317	338	345	355	rVB	239841	368113	47.82%	4.613%
2	5.793	420	426	439	rVB	337595	553844	71.94%	6.940%
3	7.408	694	701	712	rBV	441244	768138	99.78%	9.626%
4	8.272	841	848	854	rBV	137400	226945	29.48%	2.844%
5	9.441	1040	1047	1055	rBV	269253	484313	62.91%	6.069%
6	10.846	1279	1286	1295	rBV3	18530	36901	4.79%	0.462%
7	11.104	1323	1330	1337	rBV	182812	322515	41.89%	4.042%
8	13.513	1732	1740	1746	rBV	361180	560086	72.75%	7.019%
9	14.882	1966	1973	1981	rVB	287365	448070	58.20%	5.615%
10	15.276	2036	2040	2049	rVB6	3513	9334	1.21%	0.117%
11	15.687	2101	2110	2114	rVB5	7612	15009	1.95%	0.188%
12	16.092	2172	2179	2184	rBV2	9491	16489	2.14%	0.207%
13	16.357	2219	2224	2234	rBV	358176	547414	71.11%	6.860%
14	16.568	2253	2260	2266	rBV	25742	47468	6.17%	0.595%
15	16.944	2318	2324	2328	rVB7	6397	11715	1.52%	0.147%
16	17.338	2387	2391	2395	rBV3	8350	10721	1.39%	0.134%
17	17.391	2395	2400	2406	rBV	36975	57804	7.51%	0.724%
18	17.614	2432	2438	2444	rBV	382034	552864	71.82%	6.928%
19	17.996	2499	2503	2507	rVB2	10973	15357	1.99%	0.192%
20	18.072	2513	2516	2523	rVB5	9522	15147	1.97%	0.190%
21	18.213	2537	2540	2542	rBV3	7495	9266	1.20%	0.116%
22	18.243	2542	2545	2550	rVB2	21175	26835	3.49%	0.336%
23	18.384	2564	2569	2570	rBV5	11915	17717	2.30%	0.222%
24	18.466	2579	2583	2590	rBV3	34493	57046	7.41%	0.715%
25	18.754	2629	2632	2638	rVB6	9884	15191	1.97%	0.190%
26	19.206	2706	2709	2714	rVB3	10597	15755	2.05%	0.197%
27	19.400	2739	2742	2747	rVB4	20217	23347	3.03%	0.293%
28	19.647	2780	2784	2790	rVB	18781	30132	3.91%	0.378%
29	19.723	2793	2797	2802	rBV5	16158	25641	3.33%	0.321%
30	19.941	2831	2834	2837	rBV	12942	13264	1.72%	0.166%
31	19.976	2838	2840	2843	rVV4	13103	18552	2.41%	0.232%
32	20.005	2843	2845	2852	rVB	20493	26794	3.48%	0.336%
33	20.188	2871	2876	2882	rVB	613569	769841	100.00%	9.647%
34	20.470	2920	2924	2929	rBV2	16889	23790	3.09%	0.298%
35	20.605	2941	2947	2953	rBV2	41248	88125	11.45%	1.104%
36	20.969	3004	3009	3018	rVB	28685	61112	7.94%	0.766%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124055

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.492	3094	3098	3113	rVB3	54402	135201	17.56%	1.694%
38	21.745	3138	3141	3147	rVB2	13522	18459	2.40%	0.231%
39	21.891	3159	3166	3173	rBV2	410224	710351	92.27%	8.902%
40	22.056	3191	3194	3198	rVB	19498	25705	3.34%	0.322%
41	23.419	3423	3426	3436	rVB3	17982	32256	4.19%	0.404%
42	23.625	3456	3461	3469	rVB	29211	59073	7.67%	0.740%
43	25.288	3734	3744	3756	rVB2	244350	708314	92.01%	8.876%

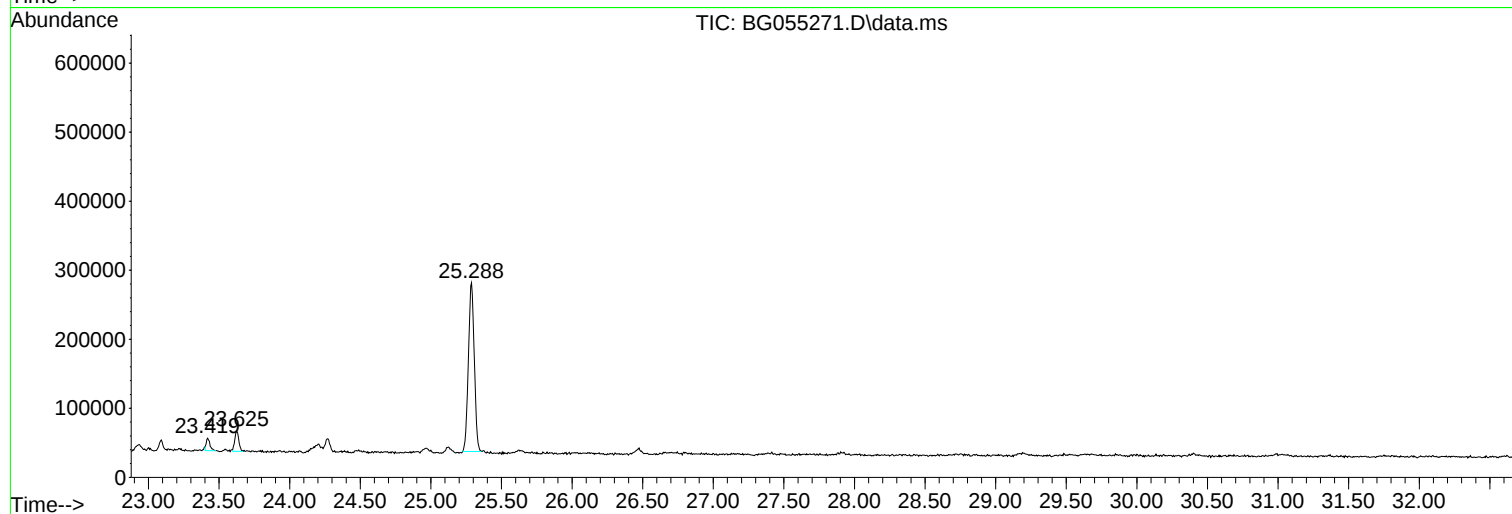
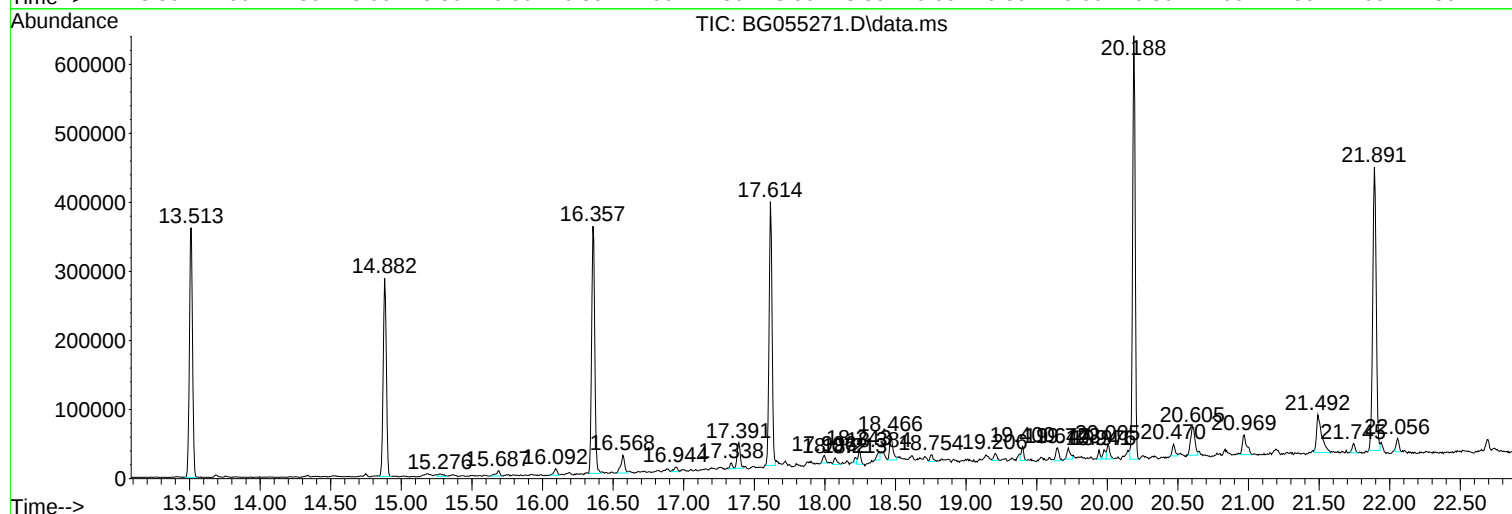
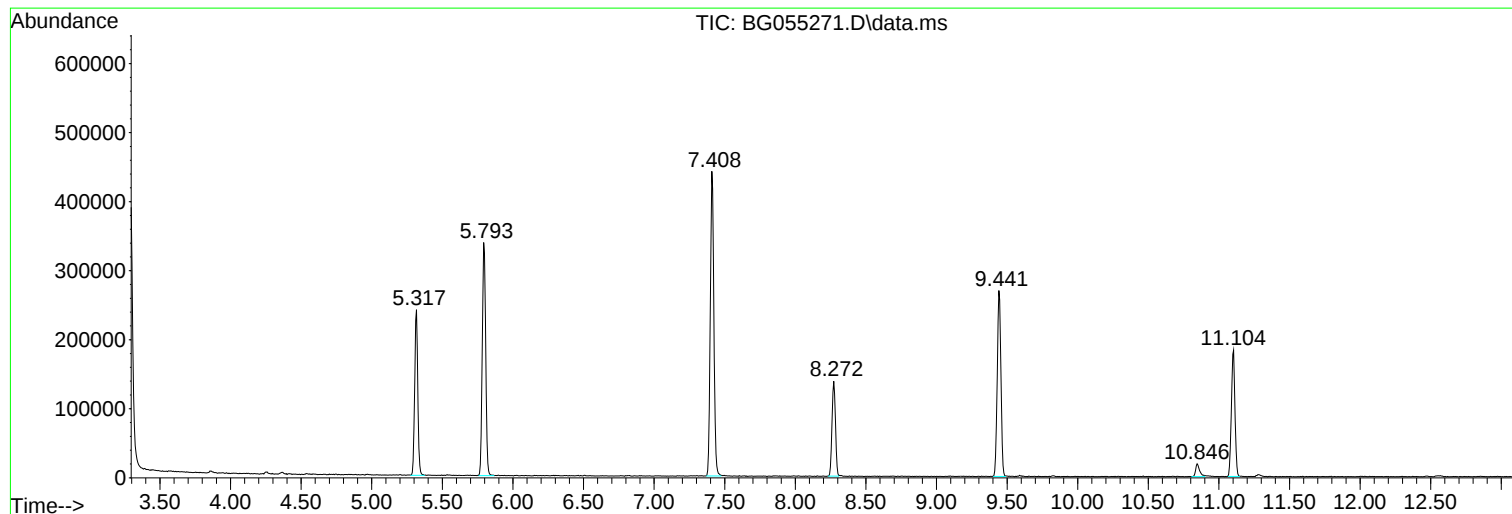
Sum of corrected areas: 7980014

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124055

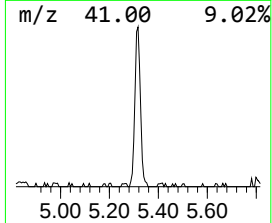
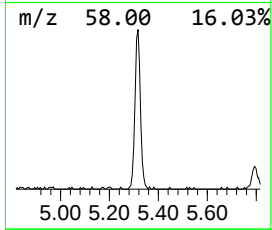
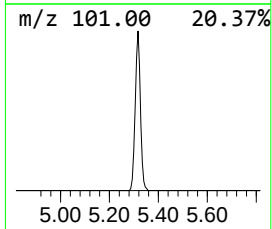
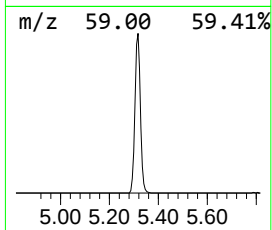
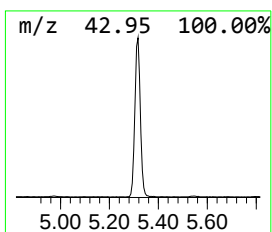
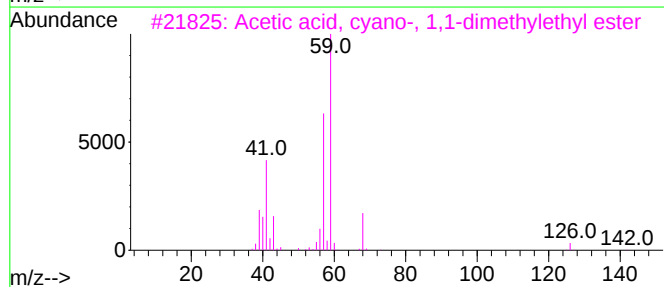
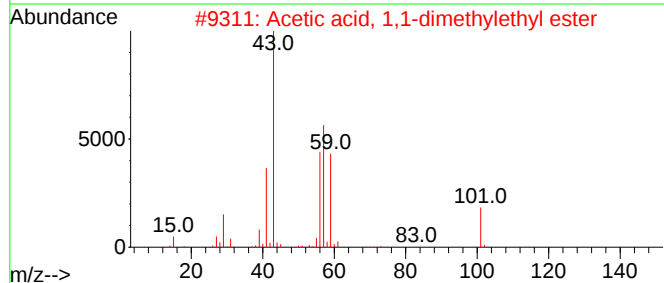
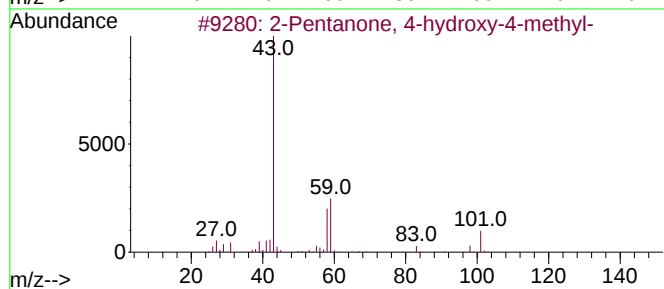
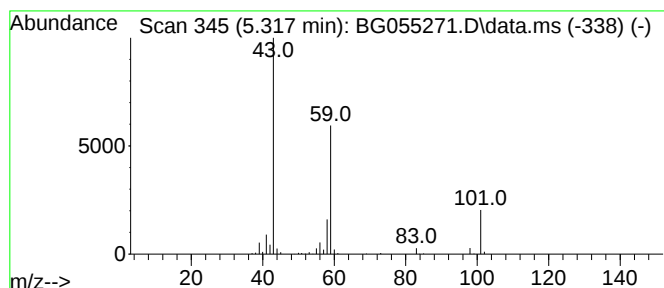
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.317	32.44 ng	368113	1,4-Dichlorobenzene-d4	8.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124055

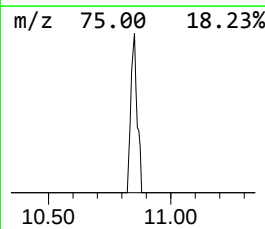
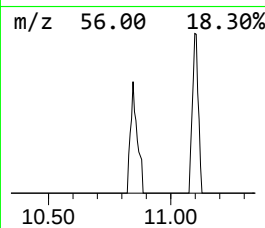
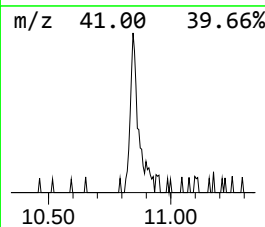
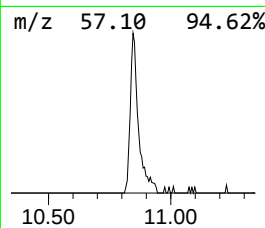
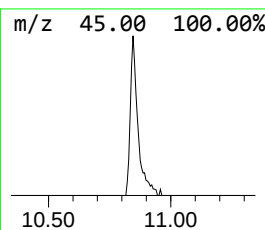
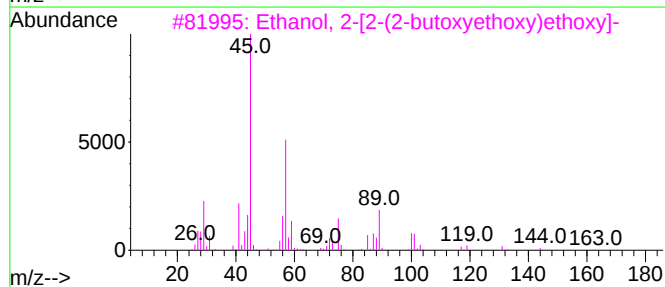
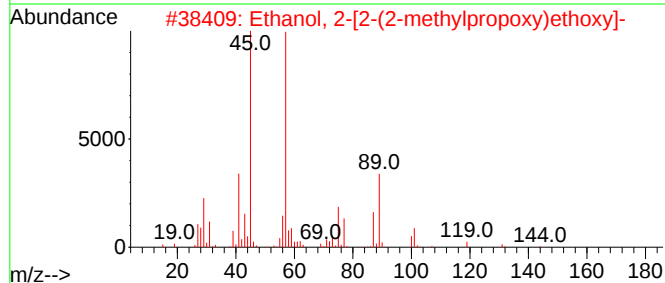
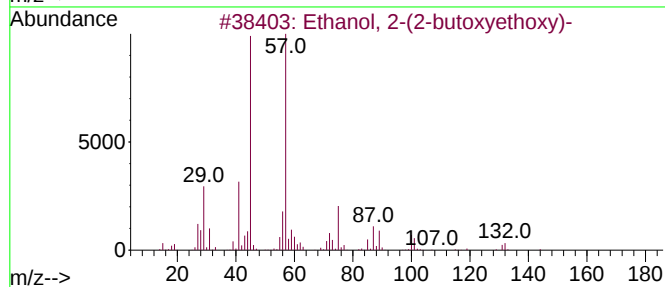
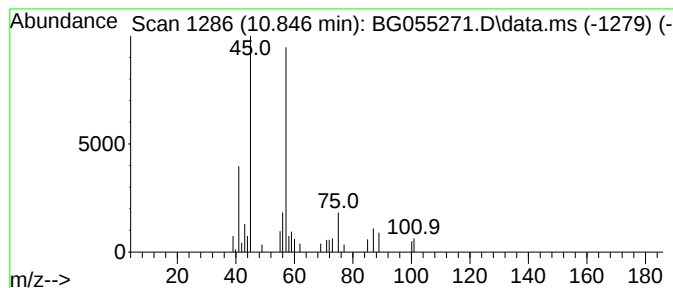
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.846	2.29 ng	36901	Naphthalene-d8	11.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	64
3			Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	206	C10H22O4	000143-22-6	50
4			Propanoic acid, 2-hydroxy-, 2-methyl-	146	C7H14O3	000585-24-0	50
5			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

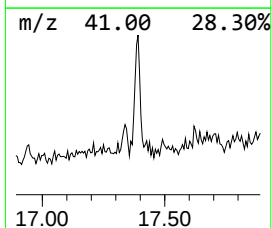
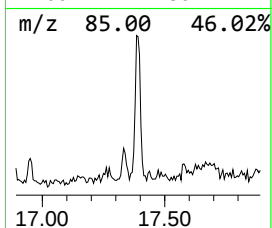
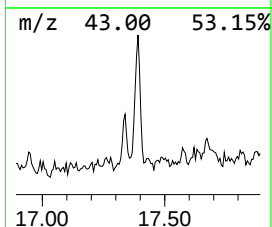
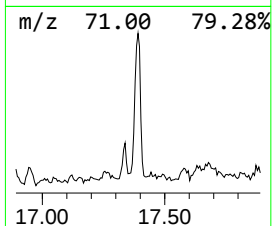
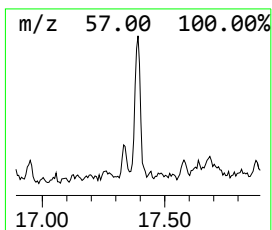
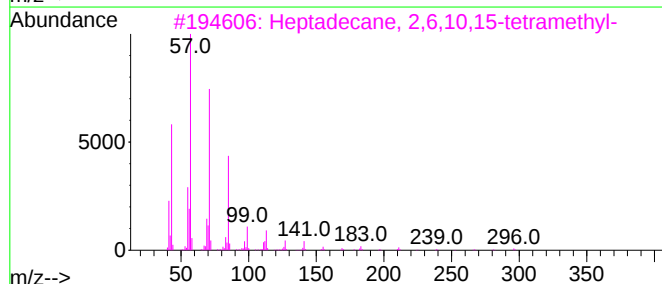
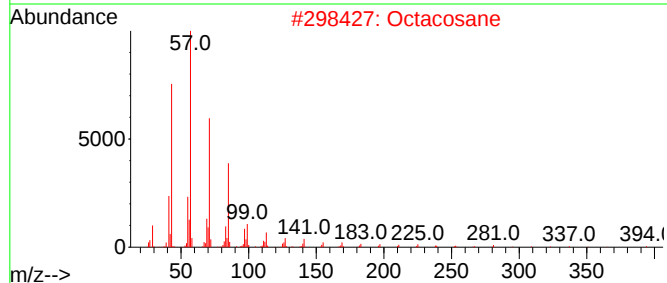
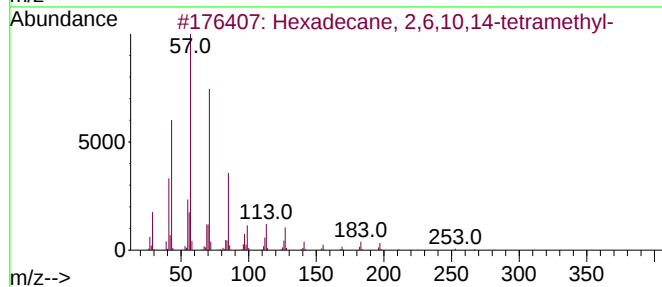
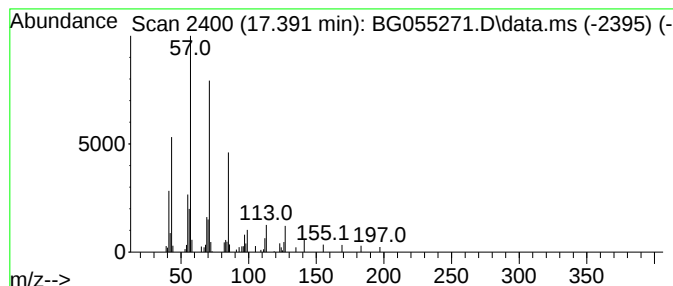
Instrument :
BNA_G
ClientSampleId :
124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.391	2.09 ng	57804	Phenanthrene-d10	17.614	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4	Tetracosane	338	C24H50	000646-31-1	80
5	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124055

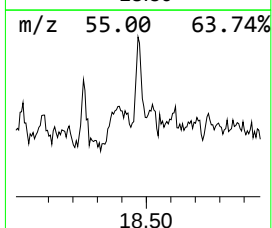
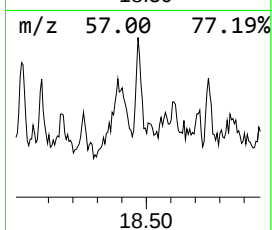
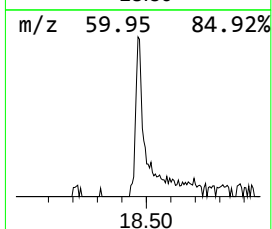
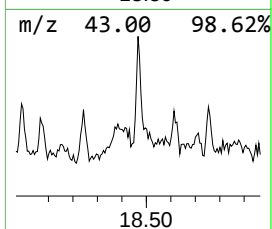
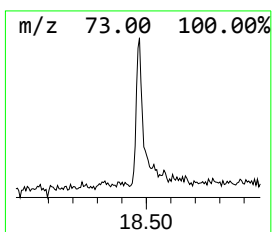
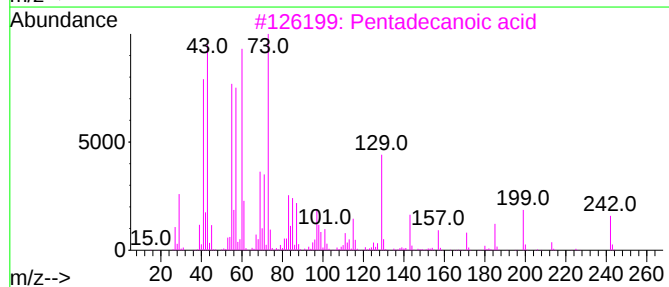
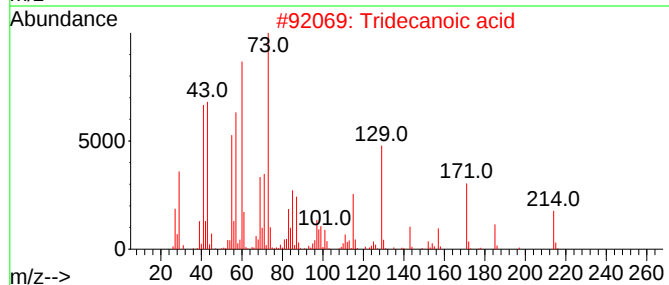
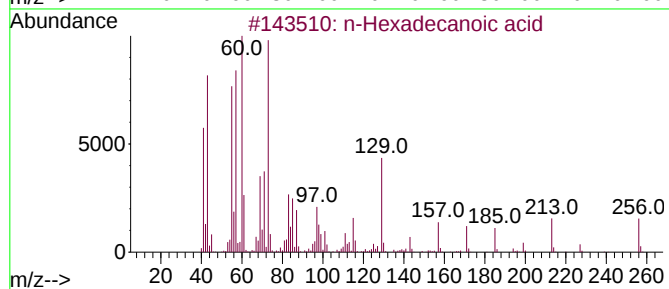
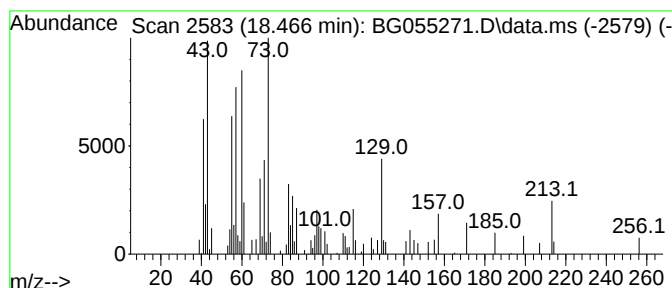
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.466	2.06 ng	57046	Phenanthrene-d10	17.614

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124055

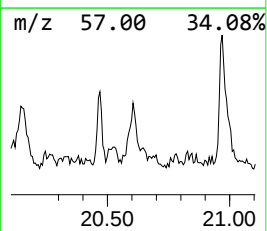
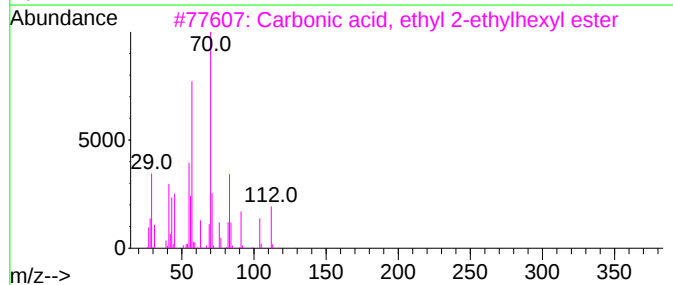
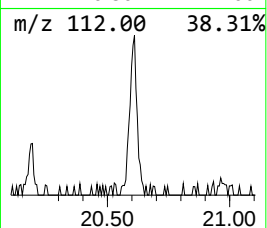
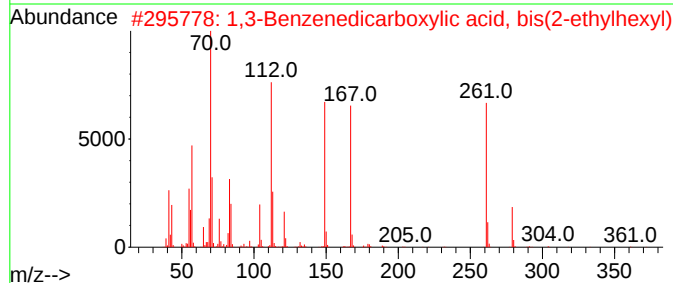
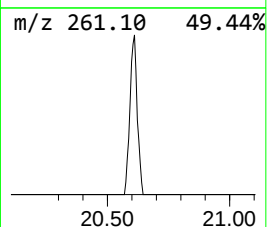
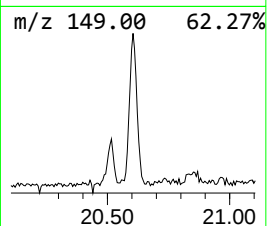
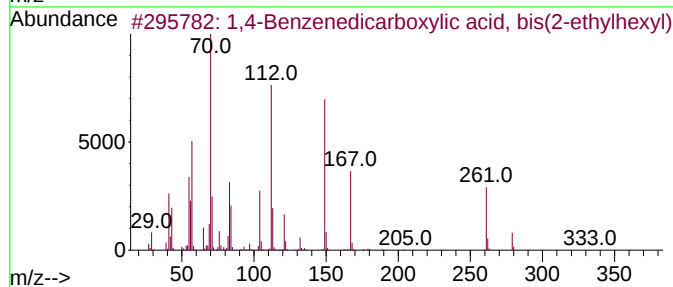
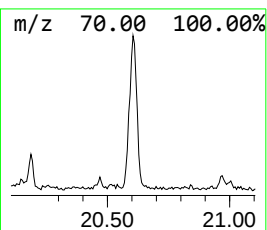
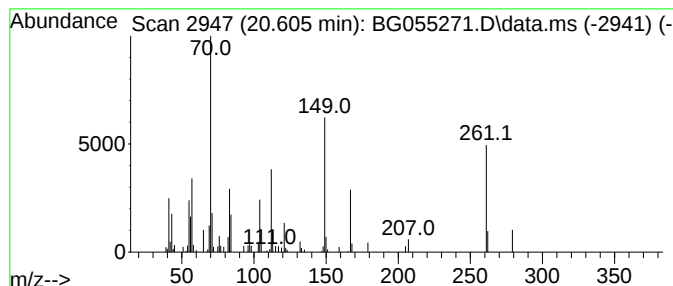
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.605	2.48 ng	88125	Chrysene-d12	21.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	53
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	50
3			Carbonic acid, ethyl 2-ethylhexy...	202	C11H22O3	1000383-13-1	32
4			6-Methyl-cyclohex-2-en-1-ol	112	C7H12O	1000144-17-3	27
5			2-Ethylhexyl acrylate	184	C11H20O2	000103-11-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124055

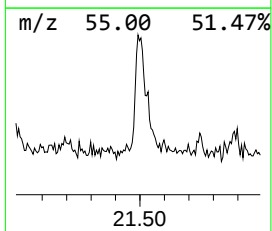
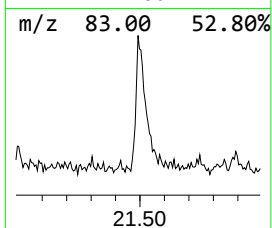
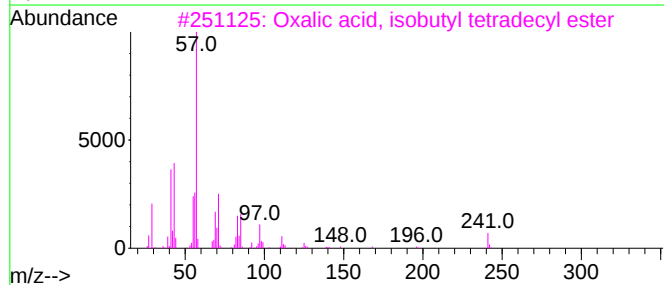
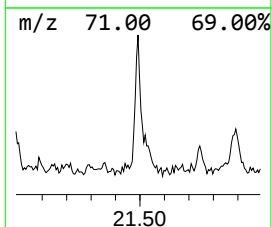
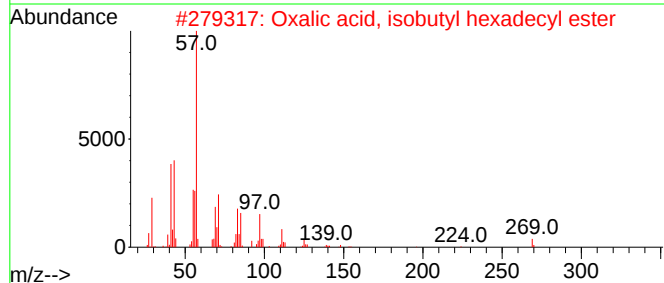
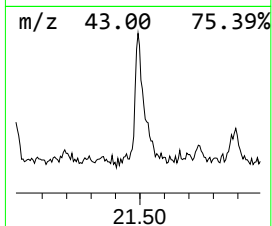
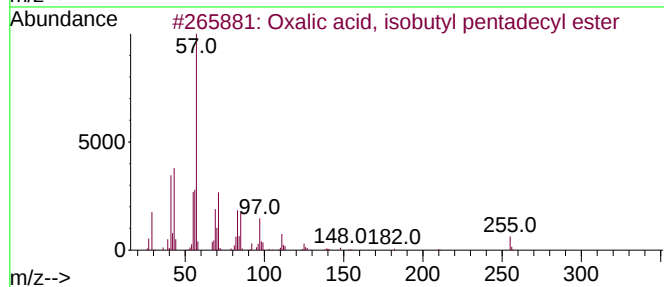
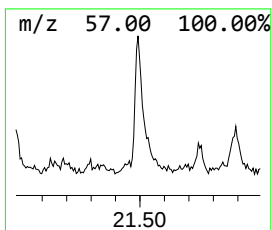
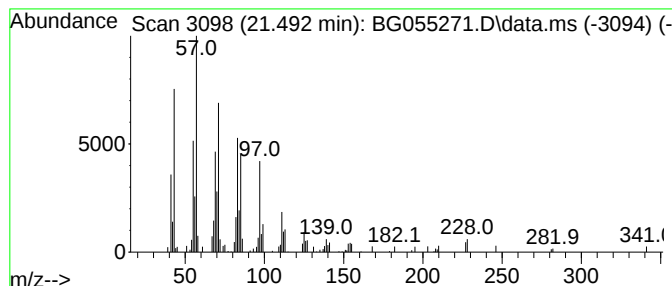
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxalic acid, isobutyl penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.492	3.81 ng	135201	Chrysene-d12	21.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
2			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
4			Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	87
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102522\
Data File : BG055271.D
Acq On : 25 Oct 2022 11:12
Operator : CG/JU
Sample : N5253-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
124055

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.317	32.4	ng	368113	1	8.272	226945	20.0
Ethanol, 2-(2-b...	10.846	2.3	ng	36901	2	11.104	322515	20.0
Hexadecane, 2,6...	17.391	2.1	ng	57804	4	17.614	552864	20.0
n-Hexadecanoic ...	18.466	2.1	ng	57046	4	17.614	552864	20.0
1,4-Benzenedica...	20.605	2.5	ng	88125	5	21.892	710351	20.0
Oxalic acid, is...	21.492	3.8	ng	135201	5	21.892	710351	20.0